

«beta»-Alanine, N-(2-furoyl)-, dodecyl ester

Inchi: InChI=1S/C20H33NO4/c1-2-3-4-5-6-7-8-9-10-11-16-25-19(22)14-15-21-20(23)18-13-12-
InchiKey: DZZVWJSSFOZTSW-UHFFFAOYSA-N
Formula: C20H33NO4
SMILES: CCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccco1
Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.27		Crippen Method
logp	4.864		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
rinpol	2718.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321982&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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